



AFRL-RX-WP-TM-2013-0156

IMPLICATIONS OF INTEGRATED COMPUTATIONAL MATERIALS ENGINEERING WITH RESPECT TO EXPORT CONTROL

**Charles H. Ward
AFRL/RX**

**SEPTEMBER 2013
Technical Memorandum**

Approved for public release; distribution unlimited.

See additional restrictions described on inside pages

STINFO COPY

**AIR FORCE RESEARCH LABORATORY
MATERIALS AND MANUFACTURING DIRECTORATE
WRIGHT-PATTERSON AIR FORCE BASE, OH 45433-7750
AIR FORCE MATERIEL COMMAND
UNITED STATES AIR FORCE**

NOTICE AND SIGNATURE PAGE

Using Government drawings, specifications, or other data included in this document for any purpose other than Government procurement does not in any way obligate the U.S. Government. The fact that the Government formulated or supplied the drawings, specifications, or other data does not license the holder or any other person or corporation; or convey any rights or permission to manufacture, use, or sell any patented invention that may relate to them.

This report was cleared for public release by the USAF 88th Air Base Wing (88 ABW) Public Affairs Office (PAO) and is available to the general public, including foreign nationals.

Copies may be obtained from the Defense Technical Information Center (DTIC)
(<http://www.dtic.mil>).

AFRL-RX-WP-TM-2013-0156 HAS BEEN REVIEWED AND IS APPROVED FOR
PUBLICATION IN ACCORDANCE WITH ASSIGNED DISTRIBUTION STATEMENT.

//Signature//

CHARLES H. WARD
Acting Deputy Director
Materials and Manufacturing Directorate
Air Force Research Laboratory

//Signature//

JOHN W. GLOYSTEIN, Colonel, USAF
Acting Director
Materials and Manufacturing Directorate
Air Force Research Laboratory

This report is published in the interest of scientific and technical information exchange, and its publication does not constitute the Government's approval or disapproval of its ideas or findings.

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

The public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Department of Defense, Washington Headquarters Services, Directorate for Information Operations and Reports (0704-0188), 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number. **PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ADDRESS.**

1. REPORT DATE (DD-MM-YY) September 2013			2. REPORT TYPE Technical Memorandum		3. DATES COVERED (From - To) 22 January 2013 – 23 January 2013	
4. TITLE AND SUBTITLE IMPLICATIONS OF INTEGRATED COMPUTATIONAL MATERIALS ENGINEERING WITH RESPECT TO EXPORT CONTROL					5a. CONTRACT NUMBER In-House	
					5b. GRANT NUMBER	
					5c. PROGRAM ELEMENT NUMBER 62102F	
6. AUTHOR(S) Charles H. Ward					5d. PROJECT NUMBER 4347	
					5e. TASK NUMBER	
					5f. WORK UNIT NUMBER POYE (program)	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Air Force Research Laboratory Materials and Manufacturing Directorate, AFRL/RX Wright-Patterson Air Force Base, OH 45433-7750					8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) Air Force Research Laboratory Materials and Manufacturing Directorate Wright-Patterson Air Force Base, OH 45433-7750 Air Force Materiel Command United States Air Force					10. SPONSORING/MONITORING AGENCY ACRONYM(S) AFRL/RX	
					11. SPONSORING/MONITORING AGENCY REPORT NUMBER(S) AFRL-RX-WP-TM-2013-0156	
12. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution unlimited.						
13. SUPPLEMENTARY NOTES PA Case Number: 88ABW-2013-4009; Clearance Date: 10 Sep 2013. This report contains color.						
14. ABSTRACT A meeting of representatives from combined government, industry, and academia was held to evaluate the implications of Integrated Computational Materials Engineering (ICME) with respect to current export control regulations and identify recommendations for improvement. The meeting was held on 22-23 January 2013 in Dayton, OH and focused on structural materials for aerospace applications. The group arrived at a focused set of four recommended actions to overcome the friction points between ICME and export control: 1) Develop ICME case studies and export control decision trees to more fully explore the interaction of ICME with export control; 2) Create tailored and accessible export control training to educate the ICME community on export controls; 3) Implement proactive government policy to promote evaluation of export control issues at the beginning of external research efforts through contracting procedures; and, 4) Clarify export control definitions to aid determination of applicability of specific controls in an ICME environment.						
15. SUBJECT TERMS export control; ITAR; EAR; ICME; ICMSE; integrated computational materials engineering; materials; modeling; simulation; engineering design						
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT: SAR	18. NUMBER OF PAGES 20	19a. NAME OF RESPONSIBLE PERSON (Monitor) Charles H. Ward 19b. TELEPHONE NUMBER (Include Area Code) (937) 255-2738	
a. REPORT Unclassified	b. ABSTRACT Unclassified	c. THIS PAGE Unclassified				

Table of Contents

Section	Page
Executive Summary.....	1
Introduction.....	2
Stakeholder Perspectives.....	3
An Industrial Perspective on ICME.....	3
Current Export Controls.....	5
Academic Perspective.....	7
Industry Perspectives.....	8
Friction Points between ICME and Export Control.....	10
Clarity in current export controls for making determinations relevant to ICME.....	10
Adequacy of export controls in covering relevant ICME scenarios.....	10
Community barriers facing ICME in an export control environment.....	11
Potential Solutions to Overcoming Friction Points.....	12
Develop best practices and pathways to explore export control applicability & adequacy..	12
Clarifying/reinforcing current export controls.....	12
Educational Resources for the ICME Community.....	13
Recommended Actions.....	14
References.....	15
Appendix 1: Represented Organizations.....	16

Executive Summary

*"Integrated Computational Materials Engineering (ICME) is the integration of materials information, captured in computational tools, with engineering product performance analysis and manufacturing-process simulation."*¹ This definition of ICME provided by the National Research Council describes the complexity of the engineering framework being constructed for 21st century materials science and engineering. This framework will be comprised of modeling tools and experimental and computational data to provide an integrated engineering capability that describes the composition, processing, structure, and property relationships of a material used to design and manufacture components and is used to design and manufacture components in a significantly accelerated time frame and at reduced costs.

A meeting of representatives from combined government, industry, and academia was held to evaluate the implications of ICME with respect to current export control regulations and identify recommendations for improvement. The meeting was held on 22-23 January 2013 in Dayton, OH and focused on structural materials for aerospace applications. The objective of the meeting was to determine what steps need to be taken within government and the materials science and engineering community to ensure adequate protection of this emerging technology while maintaining the necessary flow of information to continue scientific and engineering advancements.

Thirty-seven technical and export control experts representing government, aerospace prime contractors, material suppliers, software vendors, academia and professional societies participated in person or via teleconference. The first day of the meeting was structured for presentation of a wide variety of stakeholder perspectives to provide all attendees an appreciation of the key issues. The second day was spent focused on documenting the "friction points" between ICME and export control as uncovered during the first day, as well as proposing potential solutions to overcoming these friction points.

The group arrived at a focused set of four recommended actions to overcome the friction points between ICME and export control: 1) Develop ICME case studies and export control decision trees to more fully explore the interaction of ICME with export control; 2) Create tailored and accessible export control training to educate the ICME community on export controls; 3) Implement proactive government policy to promote evaluation of export control issues at the beginning of external research efforts through contracting procedures; and, 4) Clarify export control definitions to aid determination of applicability of specific controls in an ICME environment.

Introduction

*“Integrated Computational Materials Engineering (ICME) is the integration of materials information, captured in computational tools, with engineering product performance analysis and manufacturing-process simulation.”*¹ This definition of ICME provided by the National Research Council describes the complexity of the engineering framework being constructed for 21st century materials science and engineering. This framework will be comprised of modeling tools and experimental and computational data to provide an integrated engineering capability that describes the composition, processing, structure, and property relationships of a material used to design and manufacture components.

Numerous entities have observed that the complexity and significantly enhanced engineering capability of an ICME framework raise important questions pertaining to the suitability and adequacy of current export control regulations to protect US national security while allowing essential trade and exchange of scientific information. To address this concern, a combined government, industry, and academia meeting was held to evaluate the implications of ICME with respect to current export control regulations and identify recommendations for improvement. The meeting was held on 22-23 January 2013 in Dayton, OH and focused on structural materials for aerospace applications. The objective of the meeting was to determine what steps need to be taken within government and the materials science and engineering community to ensure adequate protection of this emerging technology while maintaining the necessary flow of information to continue scientific and engineering advancements.

It must be noted that this report summarizes a wide variety of inputs presented during the course of a two-day meeting. Therefore, the statements provided within cannot be taken as having been endorsed by the participants.

Stakeholder Perspectives

Thirty-seven technical and export control experts representing government, aerospace prime contractors, material suppliers, software vendors, academia and professional societies participated in this meeting (Appendix 1). The first day of the meeting was structured for presentation of a wide variety of stakeholder perspectives to provide all attendees an appreciation of the key issues. The second day was spent in working sessions primarily focused on documenting the “friction points” between ICME and export control as uncovered during the first day, as well as proposing potential solutions to overcoming these friction points.

An Industrial Perspective on ICME

A representative from a major turbine engine manufacturer provided an introductory presentation outlining a vision of ICME and how it will impact the means and processes used in industry to design and manufacture aerospace systems. Implementation of ICME will not just introduce new technologies, it will cause fairly significant shifts in culture, communication modalities, and engineering practices throughout the entire ICME supply chain to include prime contractors, materials suppliers, software vendors, materials testing entities, academia, professional societies and government organizations. The key elements of an implemented ICME framework include:

- Physics-Based Materials Mechanism Understanding – advances here will provide the most robust basis for predictive capability in computational models.
- Computational Models – provide the means to quantitatively and consistently employ captured materials and processing information.
- Digital Materials Data – the primary form by which specific materials and processing information will be conveyed across the ICME supply chain.
- Process Models
- Process Boundary Conditions – requires a means by which required information can be exchanged across supply-chain boundaries while protecting intellectual property.
- Material and Process Simulation and Outputs
- Supply-Chains – from integration of computational models to aggregation of digital data along the materials development, manufacture, deployment and sustainment phases of a materials lifecycle, all adding value to the final product will participate in an integrated supply chain.
- Product Data
- Specifications
- Linkages of Materials/Process Models with other Engineering Disciplines (Design, Structures, Performance)

The targeted benefits from industrial implementation of ICME are significant and far reaching throughout the product life-cycle. It is anticipated that reduced product development cycle-time and costs will result when both design and process engineers are able to use modeling tools as part of standard engineering practice in place of shop-floor trials. This migration will build toward a “Right-the-First-Time Development” environment (Figure 1). ICME will also lead to a reduced cost of product quality. A reduction in component testing will be enabled

through improved product and process modeling capabilities; while reduced scrap and rework throughout the supply chain will result in a “First-Time Yield of One” in new product manufacture. Finally, it is envisaged that ICME will improve and optimize material performance, resulting in improved component capabilities through reduced property scatter and location specific design as well as utilization of low cost alternatives to expensive alloys.

Current engineering practice defines an aerospace product in terms of Mechanical Properties (as a function of chemistry and microstructure), Microstructure (as a function of chemistry and processing), and Processing (as a function of component geometry). The artifacts of this practice include traditional engineering definitions of materials expressed through empirical and data driven design curves, specifications, prints notes, and fixed process requirements. Implementation of ICME will require a shift to a ‘model based definition’ of a material. Defining material equivalency and methods to differentiate material of one control pedigree from another is required for component design. The requirements for successful model application include: Appropriate models (understanding physics and assumptions); Valid models (valid for application and specific material/process conditions); Input data requirements (appropriate material and process boundary conditions); and, Modeling system quality control (benchmarking, data/model traceability).

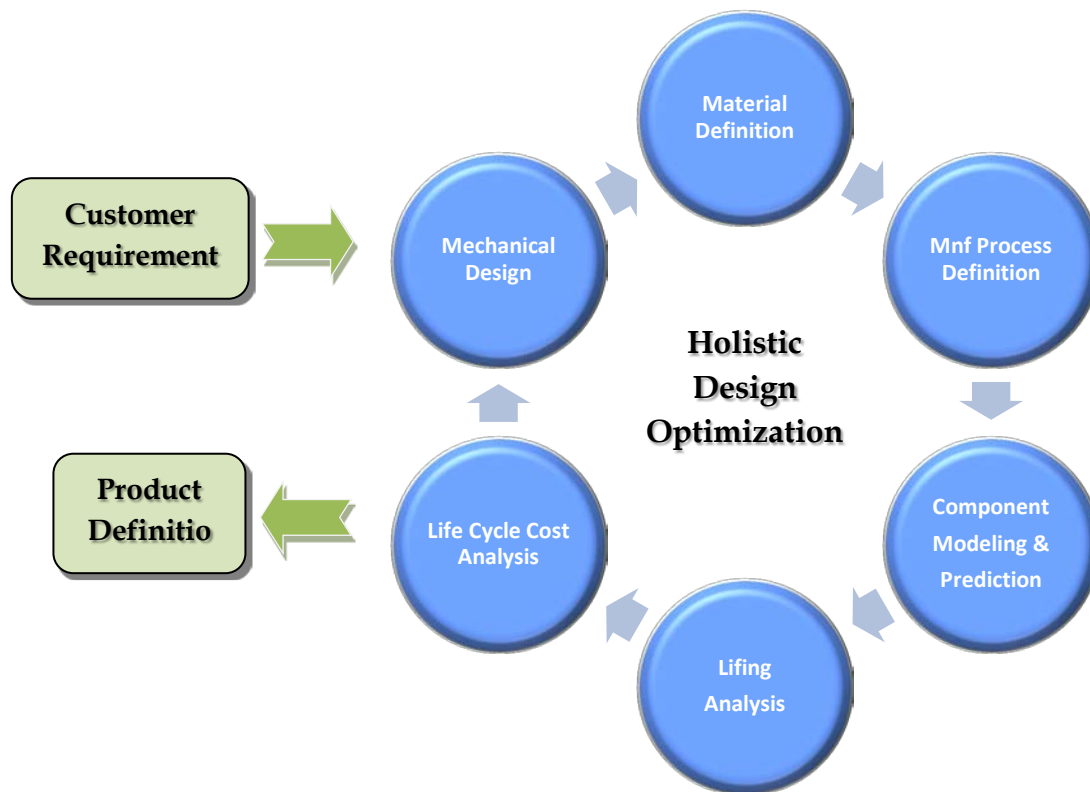


Figure 1. An ICME paradigm showing the linkages with other engineering activities.

While there are anecdotal examples of ICME use in industry within individual companies or for specific isolated examples, the successful and wide-spread implementation of ICME

throughout the aerospace supply chain is still some years off. The community will be able to credibly claim success in ICME implementation when all the following have been accomplished: 1) Develop Simulation Tools that Emulate Reality; 2) Develop Analytical Tools that Provide Insight to Material - Process - Property Relationships; 3) Implement Tools for Manufacturing Benefits; 4) Decisions Made Based on Modeling Results; and, 5) Tangible Improvements Seen Based on Decisions and Process Changes.

There are serious challenges in establishing and maintaining a sustainable ICME supply-chain in true ICME deployment. Some of the critical issues include: Physics-based model development; Alignment of university research toward industry-wide ICME goals; Clear approaches for transferring models from academia to industry (IP, Knowledge Capture, etc.); Establishment of a common, standard framework for linking mechanistic materials models, process models and design (geometry, application assessment models, etc.); and, Health of the supply-chain by providing a WIN-WIN structure.

Significant benefits can be derived from the application of computational tools to material, process and component design optimization. Holistic integration of computational materials and manufacturing models with component design functions enables global optimization for system-level improvements. Key questions that might be used in measuring ICME implementation progress include:

- Are Suppliers Encouraged or Required to Model and Validate Processes?
- Do Prints/Purchase Orders Call-Out Modeling?
- What models, data, tools are required to be shared between customers and suppliers to enable ICME?
- How do we continue to advance and apply ICME in a GLOBAL research, engineering and manufacturing world?

Current Export Controls

Representatives from the Office of the Deputy Undersecretary of Defense for Policy (Defense Technology Security Administration), Department of Commerce (DOC) (Bureau of Industry and Security), and Department of State (DOS) (Directorate of Defense Trade Controls) each presented overviews of the export control process and specifics of current controls on materials, processes, and component technologies. The two U.S. regulations governing export control are the International Traffic in Arms Regulation (ITAR)² and the Export Administration Regulation (EAR)³. These two regulations are fundamentally different in their basis for control, construct, level of description, and regulatory oversight. If an item or technology is controlled by the ITAR or EAR, an export license is required to provide the item or information to a foreign entity. It was noted that currently the approval rates for export licenses exceed 90%. Of interest, the Militarily Critical Technologies List (MCTL), formerly used to inform the export control process, and assembled by the Institute for Defense Analyses, is no longer actively maintained by DoD. As a note to the reader, the following narrative is an incomplete summary of current export control restrictions and interpretations. Many more details are provided in the regulations and the reader is strongly advised to refer to the regulations when examining specific situations.

2,3

The Department of State has statutory governance authority for the ITAR. The ITAR maintains the US Munitions List (USML) in Section 121 of the regulation, which is unilaterally defined by the US Government and contains an illustrative list of items and technologies designed specifically for military use. The technologies covered by the USML are generally described at a very high level, with many technologies being controlled through derivation from higher level descriptions. For example, turbine engines for military aircraft are a controlled item under Category VIII; therefore the specific materials and processes (and associated specific technology & data) used to create the military end item may be controlled. If applicability of ITAR to an item is in doubt, a Commodity Jurisdiction (CJ) from DOS may be requested by a potential exporter. If an item is determined to be covered by ITAR, future removal of the item from ITAR control requires Congressional notification. ITAR does contain a Public Domain exclusion from licensing for information, but this is generally limited to information already publically published, cleared by an appropriate US Government review authority, or as a product of fundamental research at a US institution of higher learning (per the ITAR definition of fundamental research). It should be noted that at the time of this meeting, the USML was undergoing revision in its structure.

The Department of Commerce has statutory authority for the EAR. With some exceptions, all items within the US, moving through the US, or of US origin regardless of location are subject to the EAR. The EAR controls specific items and technology that have dual use (military and civilian) through the Commerce Control List (CCL). The CCL is an exceptionally detailed list of restrictions divided into ten categories, of which Category 1-Special Materials and Related Equipment, Chemicals, "Microorganisms," and Toxins; Category 2-Materials Processing; and, Category 9-Propulsion Systems, Space Vehicles and Related Equipment, are most relevant to structural materials for aerospace applications. These three categories are comprised of nearly 200 pages describing restricted items and technology. In contrast to the USML, which is unilaterally set by the DOS, the CCL is primarily the product of negotiation between the 40 other member countries in the Wassenaar Arrangement, as well as other multi-lateral regimes.⁴ The DOS leads the Wassenaar Arrangement negotiations, but the US Government input is informed through a number of agencies including DOD, DOC, DOE, DHS, etc. Industry in particular plays a significant role in the Technical Advisory Committees chartered by DOC for input. The minimum process cycle time that an item could be placed on and then removed (if deemed no longer controlled) from Wassenaar Arrangement controls is six years, if every step is perfectly executed. Practically, if one wants an item added to the list, plan on it being there for a very long time. The underlying principle in EAR control is that industry has a vested interest in protecting its intellectual property. Thus, the public domain exceptions for EAR controlled items are substantively different from the ITAR. Under the EAR, the transaction of unilaterally placing information in the public domain makes the information no longer subject to the EAR, and no longer requires a license for export. Of course, this presumes the entity controlling the information authorized the individual to place the information in the public domain. The repercussion for unauthorized release is legal recourse between the two parties if an agreement controlling any release existed. The regulations provide specific definitions for public release and other terms, which must be understood to fully interpret the EAR restrictions and controls.

The discussion accompanying the presentations was lively and informative. The themes of most conversation centered on judging applicable controls in terms of technical thresholds and designed purpose for the item in question. Describing the issue in terms of technical thresholds,

where an item exceeds a well specified level of performance, is most relevant to the CCL. Thus, the components, production equipment, material, software, and technologies associated with a specific materials-related technology that exceeds a threshold defined in the CCL may be controlled. For example, the specific technical data associated with a controlled material used as input to a process model may be controlled whereas the software itself may not be controlled if it meets certain criteria such as being in the public domain or not specially designed for the application. However, if you specifically modify the model to enable design of a material that would now exceed a performance threshold, then the model itself is likely controlled. Most of the dialogue examined the meaning and applicability of the definitions used in the EAR, notably “required”--and its supporting term “peculiarly responsible”--and “specially designed”. It is not possible in this document to examine all relevant ICME scenarios when exploring applicability of export controls. Whereas the CCL is more dependent on controls set through performance thresholds (though not exclusively), the USML is more dependent on the original design intent for the item. Thus, borrowing the groupings used in the CCL, the components, production equipment, material, software, and technologies that are specifically developed for use in the design or production of a military system are most likely controlled, regardless of a threshold of performance.

Academic Perspective

The internal efforts of one major university system to stay compliant within the export control restrictions were described. It is evident that the large research universities provide freely accessible and substantive information to inform their faculty on the export control boundaries applied to university efforts. In summary, if funding entities (government or private) elect to sponsor research projects at a university without requiring publication review for restriction based on national security concerns, university researchers have the latitude to publish the results of their work in the public domain free from export controls. In fact, many larger research universities have explicit policy barring acceptance of research funding that carries restrictions on publication that would evoke export controls. Furthermore, in the context of export control, there is an emphasis placed on placing all university software, databases, and technical data in the public domain. The university also advises its staff to ask for any ECCN that may be associated with a procured software package in order to understand the status of any export controlled material it may be receiving.

Several benefits of employing ICME within the academic environment were highlighted including opportunities for exploring new processes for known materials, incremental changes in materials or process, and qualitatively new materials. It was pointed out that for ICME to enhance industrial competitiveness, many gaps that require university – industry – government collaboration must be filled. For example, universities are specifically very well suited to provide: Fundamental physical models – processing, structure, properties; Cross-disciplinary advances in computation (GPUs, algorithms), informatics; and, Advanced characterization techniques, including 3-D aspects. Finally, it should be recognized that the changes in educational paradigms needed for ICME will be driven by industrial needs and federal programs.

Given university sensitivities to export control and intellectual property, agreements on the data provided to and expected from universities in the course of industrially sponsored research should be resolved at the outset of any effort. It was noted that journals and government policies are increasingly expecting researchers to provide the data used in validation of a model when publishing. The question naturally arises as to what data will be used for validation and how will it be used in the publishing process. It’s recommended that wherever possible,

validation data should be generated at the university. In order to avoid revealing too much processing information through accompanying metadata, it was suggested that mapping out parametric analysis space would be an appropriate approach. Finally, funding entities and faculty need to plan more deliberately for moving software and models beyond campus.

Industry Perspectives

A large fraction of the participants of the meeting are members of the Metals Affordability Initiative (MAI). MAI is a public-private partnership between the US Air Force and 18 private companies representing the majority of the aerospace's specialty metals industry. MAI is targeted at development of metals technology to specifically support Air Force systems, and is executed through a Technology Investment Agreement (TIA). However, consortium members co-fund development efforts and seek the ability to apply resulting technology to subsequent commercial applications. It was noted that the language in the current TIA directs automatic application of an ITAR control statement on all MAI documents not yet cleared for release. This practice has since been stopped for more recent contracts as the DoD does not have the authority to make an export control determination. The first industrial talk raised several export control scenarios and questions encountered through the MAI TIA.

- MAI ICME projects are aimed at developing tools for specific alloys. Does the potential application of models to specific products that exceed threshold properties make the models restricted to the same level?
- MAI modeling projects are aimed at simulation of manufacturing processes that have export controls. How should the models (generic models applied to specific examples or specific models specially developed for specific examples) that could support export controlled processes be handled?
- MAI modeling efforts are being pursued to establish and formalize “industry-standard” validation methods. Is the know-how to validate models for specific applications restricted? Models could be developed and validated for parameters that could be export controlled, even though these processing parameters are not provided with commercial models. Is this level of development/validation an issue, since process windows might be rapidly “learned” through digital experimentation?
- Materials and process modeling requires unique data; often dynamic, in-process data relative to microstructure, properties and process boundary conditions. Defining methods for data generation may provide insight into critical parameters for processes.
- Input data for models and materials data in general requires specific information that defines the pedigree of this material. When does pedigree information (grain size, precipitation size, level of porosity, defects, cooling rate, strain, strain-rate, thermal history, etc.) provide “know-how” and become export controlled?
- There are many types of outputs from materials and process models, including geometry, microstructure, mechanical properties, various discriminators of “quality” and specific

transient parameters. When does predicted, virtual data become controlled? The information from models provide engineering guidance for material, process and component improvement, but it is correct to say they are not required to attain goals, as traditional Edisonian (trial-and-error) methods will work and have to this point in industry?

- Models can transform input data, which can be of various export control levels, and provide new, transformed data. If EAR ECCN 9E991 data is input into a model, is the output data controlled by the input data control levels, the model control levels or both?

Representatives from other companies provided their perspectives on export controls. Reliance on protecting one's IP as a first line of defense to controlling the flow of "knowhow" was espoused as common theme among presentations. From a materials supplier perspective, emphasis should be placed on examining practices for ensuring coverage under export controls when 'plug in' software modules are developed with government funding. From a software vendor's perspective, care must be taken in mixing controlled data with a larger body of data lest one "poison the well", and that care must be taken even in advising a client on combining different elements of a code to help solve an issue. Both situations may change the character of control for the item/service. Models and codes that provide users with direction on what specific material and process information is required to perform simulations can provide "know-how" that was learned through many years of material or process technology development.

It was clearly evident during these presentations that the larger defense contractors are much better equipped to deal with export control issues than smaller companies. This is likely due to their closer tie to the final (defense oriented) product, and their access to sufficient and trained specialists in export control. That being said, it is also clear that the regulations on materials data and computational methods related to ICME may not be the easiest to interpret by any organization. The smallest companies represented were much less versed in export control regulations, and/or expended a far greater percentage of resources to ensure compliance. One small software company provided as an example that it had expended one year's profit to obtain legal advice on applicability of export controls to its product. This exposed a unique fragility in the ICME supply chain at the small and medium size enterprise level, which make up a significant portion of the overall ICME supply-chain. Additionally, with a significant number of software companies being foreign owned, and the US export controls being more intricate and stringent than foreign regulations (e.g. deemed exports and re-export), a barrier to U.S. market entry can be envisioned. It can be anticipated that an ICME-enabled supply chain might create tensions between entities with differing products and business models that may affect the underlying premise of the EAR on companies protecting their IP.

Friction Points between ICME and Export Control

The participants of the meeting were assigned to groups to identify the key friction points between ICME and export control. Participants were distributed to maximize perspectives in each group. The following is a summary of the friction points identified by the groups and organized in themes:

Clarity in current export controls for making determinations relevant to ICME:

- The existing EAR definitions of “specially designed” and “required” are particularly ambiguous in the context of using a model or software code in the course of development, production, or use of a material. Some groups also suggested some definitions that are currently absent would be useful including “model”, “code”, “simulation”, “simulative”, “input data”, “output data”, and “generic”.
- It is not presently clear how to treat models at the various stages of their maturity. Maturity and Validation need to be assessed relative to application. For a model to provide manufacturing input on processing parameters, it may only need to provide direction and not absolute value. Is there a level of model validation/calibration that must be achieved (a threshold) in order to say the model provides utility and therefore is subject to control?
- Is there a threshold of design intent before an item becomes controlled?
- The language describing control of software can be very broad and therefore ambiguous (e.g. 1D002).
- Roles of individuals/entities in the export control process, including who determines export controls, are not clear in the community.
- Processing controls (Cat 2) need clarification, (time, temp data inputs) given availability they have the potential to allow backing into “required” processing controls from models.
- Is ICME defined well enough for the community and regulators?
- When is it appropriate to self-classify?
- Consistency in regulations and interpretations between regulating bodies.
- “Codes for specific product or materials applications, with embedded knowledge or guidance are controlled to the level of that application (i.e. there are controls today).”

Adequacy of export controls in covering relevant ICME scenarios:

- The topic of ICME workflow {also referred to as integration or the means/know-how of linking models through length scales and engineering disciplines} was frequently cited as an area where we don’t know enough to say if adequate controls are in place.
 - Workflow can further be described as the process of combining *input data*, *models* (general purpose vs application specific for part or material or both that are controlled), *output data* (virtual material, virtual parts that exceed thresholds), and *analysis &*

interpretation (iteration and optimization methods being employed) to achieve design intent.

- Related to workflow, an open question remains concerning the status of a specific process for optimization that may drive a previously uncontrolled item over established thresholds.
- There exists a lot of “would otherwise be controlled” information in public domain due to publication of information.
- Need to classify all elements of the ICME supply chain: Classify each stack of models/integration for subject to controls.

Community barriers facing ICME in an export control environment:

- While some within the materials community are very well versed in export control considerations, there is a large segment of the materials science and engineering community that lacks awareness of export control regulations. This knowledge gap can exist across government labs, industry, and academia.
- The fear (real or perceived) of export controls can hinder collaboration across groups.
- There will always be a balance (tension) in the system between competitiveness (corporate boundaries) and national security (political boundaries).
- The cost of export control compliance can be quite high, particularly for small companies.
- Large companies may not be incentivized to help small businesses work through export control issues.

Potential Solutions to Overcoming Friction Points

For this exercise, the participants of the meeting were kept in the same groups to identify potential solutions to overcome the key friction points between ICME and export control. The following is a summary of the solution sets identified by the groups and organized in themes:

Develop best practices and pathways to explore export control applicability & adequacy:

- Develop ICME case studies to examine concrete issues in determinations
 - For example, does integration of limited controlled items in an ICME workflow need additional control?
- Develop decision tree/flow chart to analyze ICME scenarios
- Create a new technical working group for ICME and map out what the regulations mean to them, write a position paper, and ask for an advisory opinion from DOC/BIS
- Enlist consortia engagement, e.g. MAI, NNMI, to build expertise in export control process and require enhanced specific export review and marking processes as part of government contract flow-down requirements
- Modularize modeling tools as best you can, separating the application specific code from the non-application-specific code
- Plan for both IP and export control from day 1—program technology release roadmap
- Map classification of different ICME modules, including transition plan—if part of gov't activity should it be a requirement?
- ITAR/EAR/IP compliant infrastructure solutions—industrial internet, digital supply chain—control and tracking of data (put in hands of those that own it)
- Government-populated database
- Infrastructure- FEPs (best practices), DARPA Vehicle Forge (Export compliant)

Clarifying/reinforcing current export controls:

- Language/definitions—sponsored by TACS:
 - Update definitions “specially designed”, “model”, “simulation”
 - Define “specific application” as realistic component design incorporating key design features required for real component: Depending on interpretation, loopholes may to exist to bypass export control intent
 - Define what “validation” means—coupon, subcomponent, or component level?

Educational Resources for the ICME Community:

- Availability of export control resources: webinars
- Develop specific targeted training packages, to include case studies
- Professional societies: reports (e.g. ICME implementation), symposia (programming), continuing education (workshops, short courses), meetings
- Publication in open literature, with data in public domain (e.g. IMMI)
- FEPs—educate and train out, get designers involved
- University courses & degrees
- Industry feedback and engagement with academic partners—affect talent pipeline.

Recommended Actions

Based on the potential solutions presented by each group, a select set of recommended actions was determined. Each of these actions will require leadership and/or participation from government, industry, and professional societies.

1. Develop ICME Case Studies and Export Control Decision Trees: A number of case studies should be constructed to more fully explore the interaction of ICME with export control. Decision trees should be developed as a universal aid in working through export control determinations. The case studies should include ample combinations of potentially controlled variables (e.g. material, input/output data, model/code/software, workflow, intended application) to adequately survey the anticipated scenarios. The creation and validation of case studies will serve multiple purposes: to highlight potential areas in the export control regulations requiring further clarification or control; serve as an educational tool; and, help develop export control decision trees/flow down tools.
2. Create Tailored and Accessible Export Control Training: Resources should be developed and made publically available to educate the ICME community on export controls. These resources could provide a basic understanding of export control through, for example, professional society publications, symposia, and websites, DOC/BIS webinars; all tailored for ICME through the case studies and decision trees developed above. Also, a forum should be established to convey ICME/export control best practices.
3. Implement Proactive Policy: Government agencies should promote evaluation of export control issues at the beginning of external research efforts through contracting procedures. R&D contracts should conduct technology transition mapping in the context of export control at the initiation of an effort to ensure clarity on disposition of data and models throughout the life-cycle of the effort.
4. Clarify Export Control Definitions: The meeting identified several areas where clarity in the export control language would aid determination of applicability of specific controls in an ICME environment. Those already defined in EAR 772 but in need of clarity include “specially designed” and “required”. Those that are not currently defined in EAR 772, but are important terms within the ICME community include ‘model’, ‘code’, ‘software’, ‘simulation’, and ‘validation’. Some of these terms, such as ‘software’, are already used in the regulation, but are not defined. Others, such as ‘validation’, are new concepts that would add clarity and may need to be incorporated into appropriate places in the CCL. This would likely be an action the DOC Technical Advisory Committees would need to champion, given the proper input.

References

- ¹. Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security (2008) The National Academies Press, Washington, DC
- ². http://www.pmddtc.state.gov/regulations_laws/itar_official.html
- ³. <http://www.bis.doc.gov/policiesandregulations/ear/index.htm>
- ⁴. <http://www.wassenaar.org/>

Appendix 1: Represented Organizations

OEMs:

GE Aviation
Honeywell
Lockheed Martin
Northrop Grumman
Pratt & Whitney
Rolls-Royce

Material Suppliers:

Howmet/Alcoa
ATI

Software Vendors:

SFTC
Thermo-Calc
Firehole Technologies
ESI

Academia:

University of California Santa Barbara

Professional Societies:

ASM International, The Minerals, Metals, and Materials Society

Government:

Air Force Research Laboratory, Materials and Manufacturing Directorate
Army Research Laboratory
Department of Commerce, Bureau of Industry and Security
Department of State, Bureau of International Security and Nonproliferation
NASA Glenn Research Center
NASA Marshall Space Flight Center
Office of the Deputy Undersecretary of Defense for Policy, Defense Technology Security Administration
Office of Naval Research